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ME469: Common Discretization Approaches: Edge-based,Vertex-Centered (EBVC)

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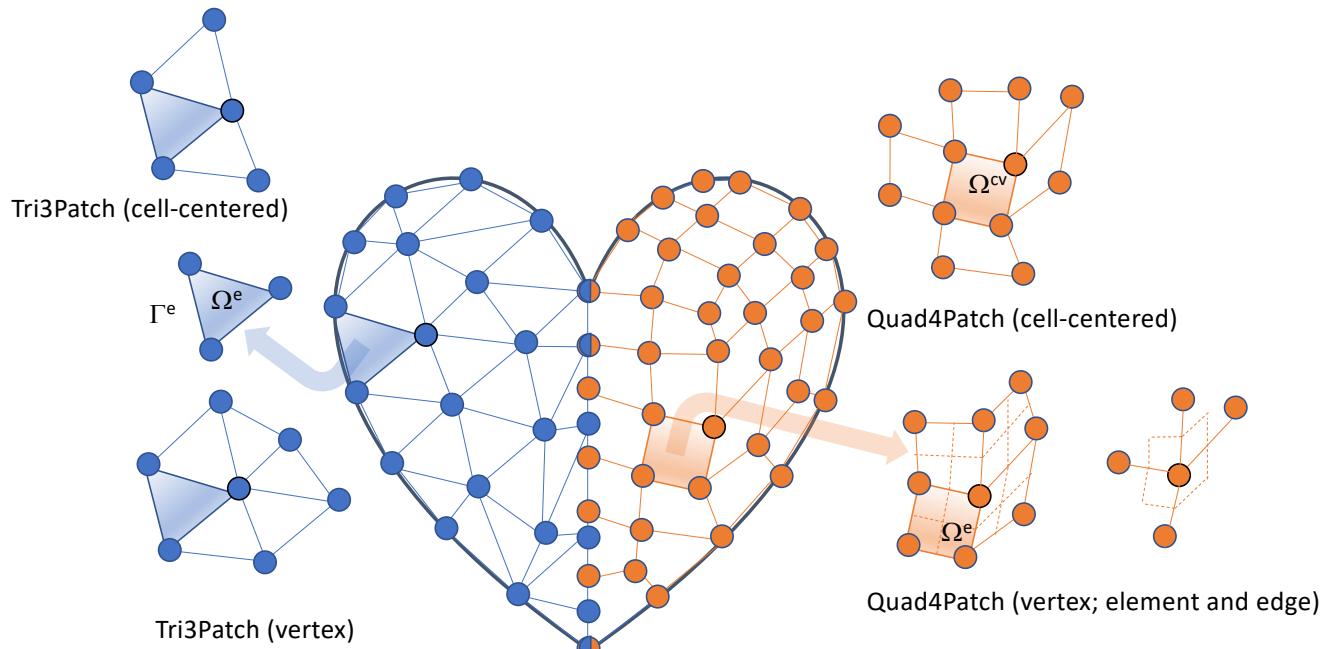
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Review of Discretization Options

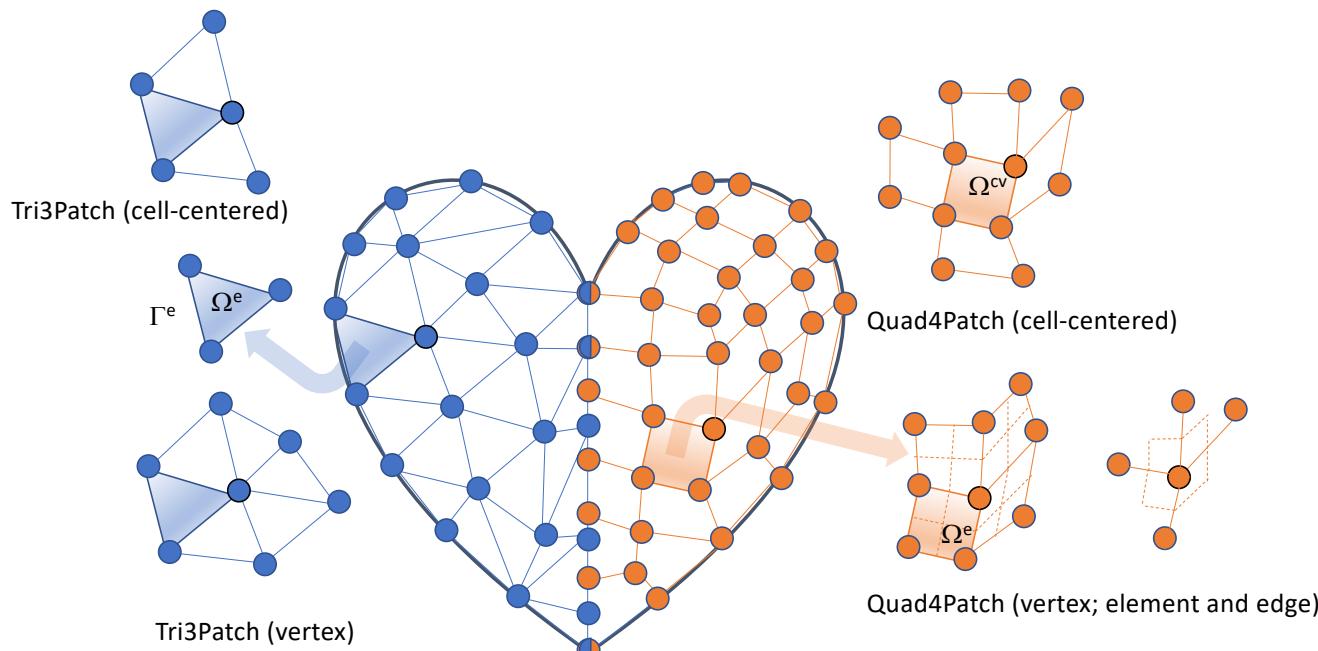
- Degree-of-freedom (DOF) for:
 - Cell-centered: Stencil is based on a element:face:element
 - DOFs at vertices of elements, or “nodes”, element:node (CVFEM, FEM), edge:node (EBVC)



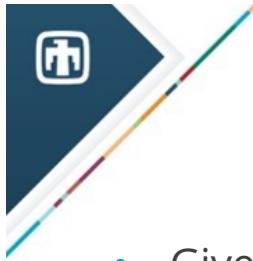


Review of Discretization Options: New, a nodal-basis...

- Degree-of-freedom (DOF) for:
 - Cell-centered: Stencil is based on a element:face:element
 - DOFs at vertices of elements, or “nodes”, element:node (CVFEM, FEM), edge:node (EBVC)



- Definition of an interpolation function:
$$\phi_{ip} = \sum_n N_n^{ip} \phi_n$$
- N_n^{ip} is the Lagrange function associated with node n
- ϕ_n is the value of the DOF at node n
- The nodal basis functions obey equipartition of unity and satisfy, $N_n^{x_j} = \delta_{nj}$



Fundamentals of Discretization: Surface vs Volume Integrations

- Given a partial differential equation (PDE) and associated volumetric form:

$$\int \frac{\partial F_j}{\partial x_j} dV = \int S dV$$

- Applying Gauss Divergence provides the standard finite volume form for fluxes in surface integral form:

$$\int \frac{\partial F_j}{\partial x_j} dV = \int F_j n_j dS \quad \longrightarrow \quad \int F_j n_j dS = \int S dV$$

- We can also multiply PDE by an arbitrary test function, w , and integrate over a volume,

$$\int w \frac{\partial F_j}{\partial x_j} dV = \int w S dV$$

$$\int \frac{\partial w}{\partial x_j} F_j dV - \int w F_j dS = \int w S dV$$

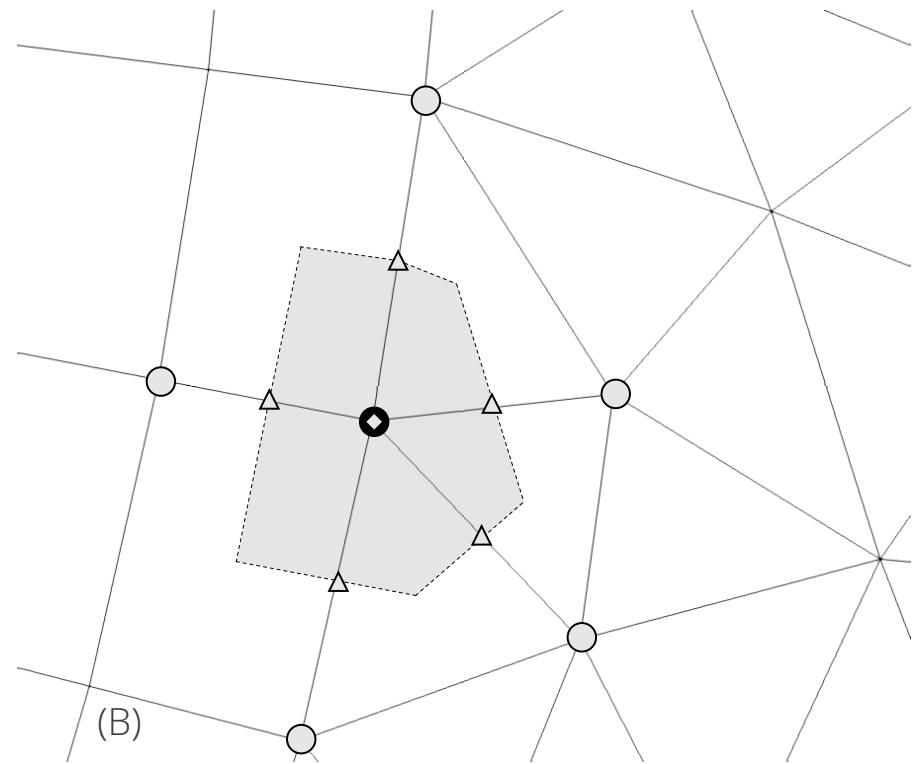
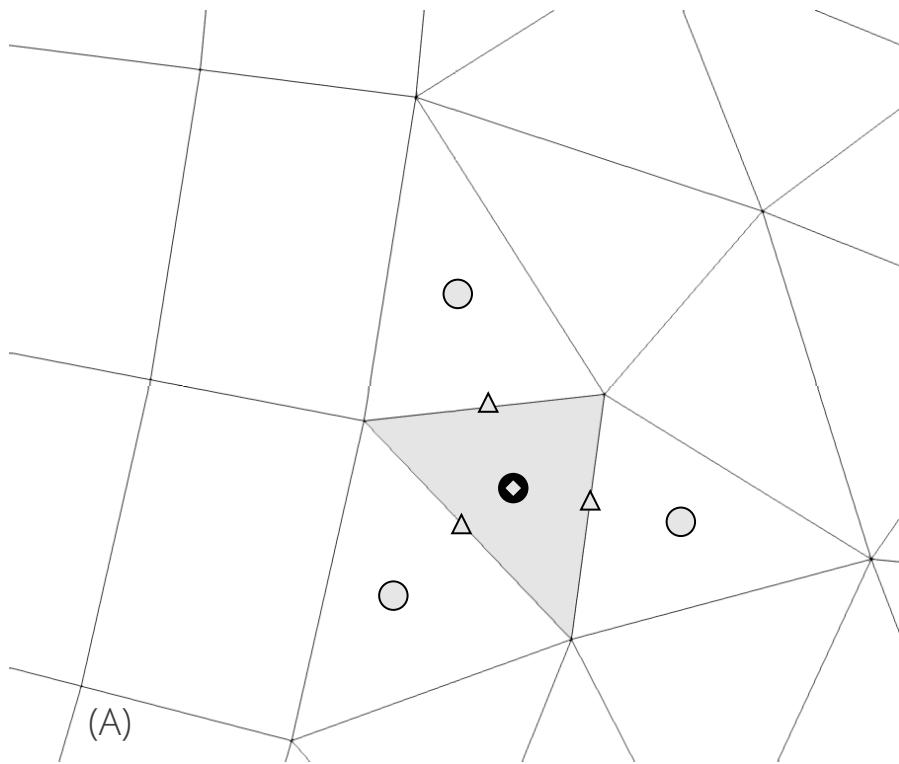
Next, integrate by parts and apply Gauss-Divergence. Note, that test function must be differentiable – shown here, at least once..

$$\frac{\partial w F_j}{\partial x_j} = w \frac{\partial F_j}{\partial x_j} + \frac{\partial w}{\partial x_j} F_j$$



Cell-Centered (CC) and Edge-Based Vertex-Centred (EBVC): Each are generally a two-state scheme, Left (L) and Right(R)

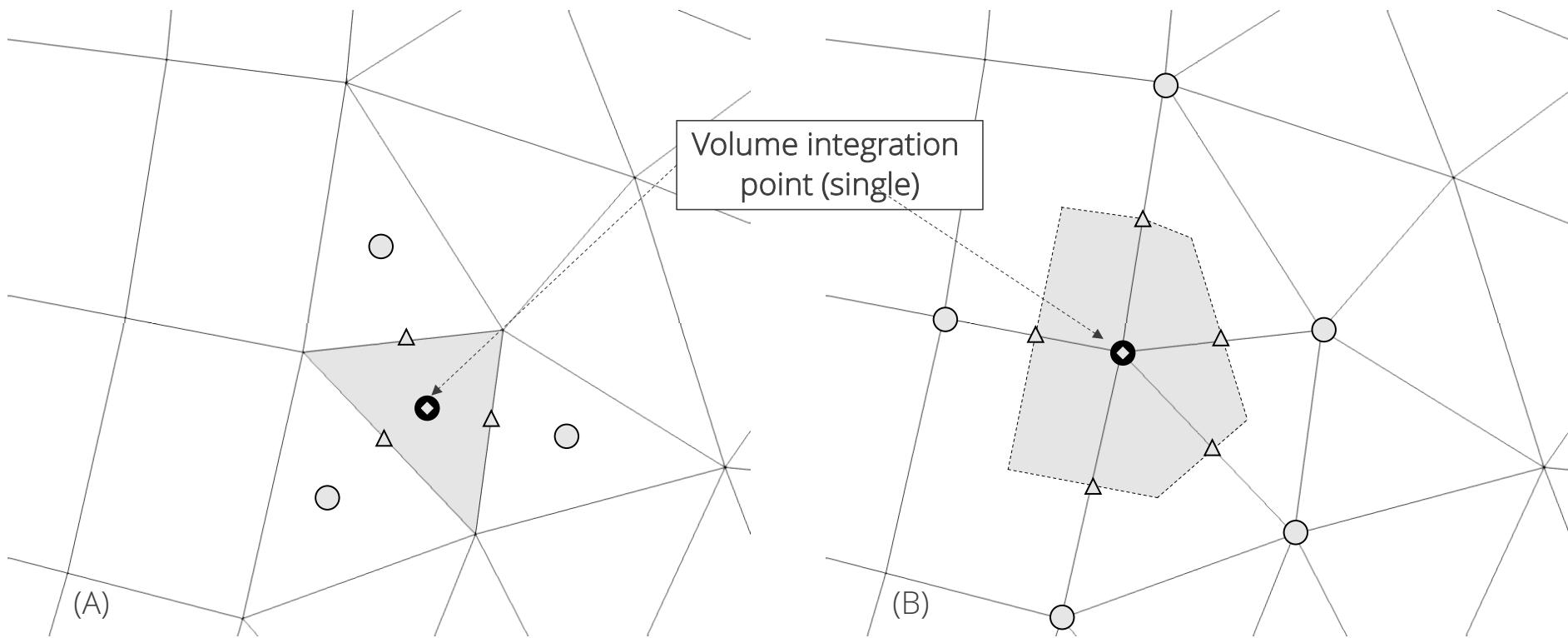
- CC (A) and EBVC (B) – As shown below, each have a set of common features
 - Class Discussion: What are the common features?





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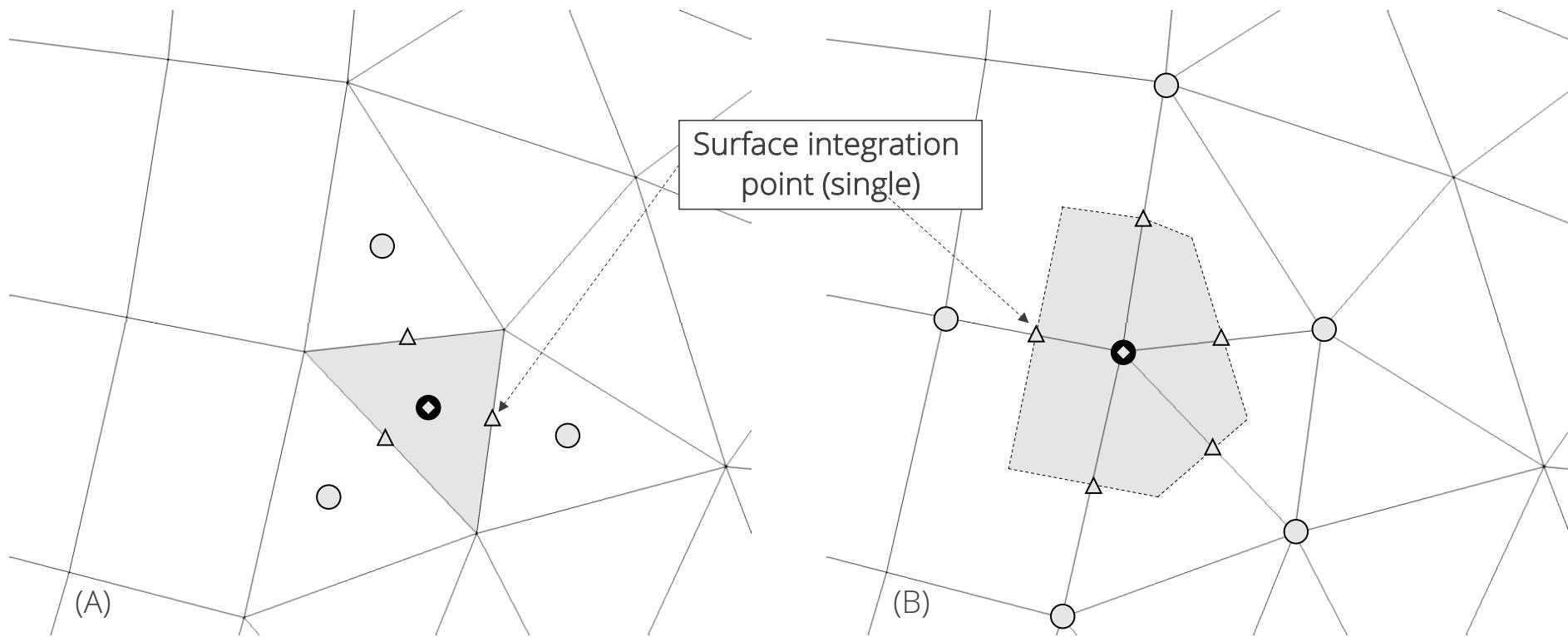
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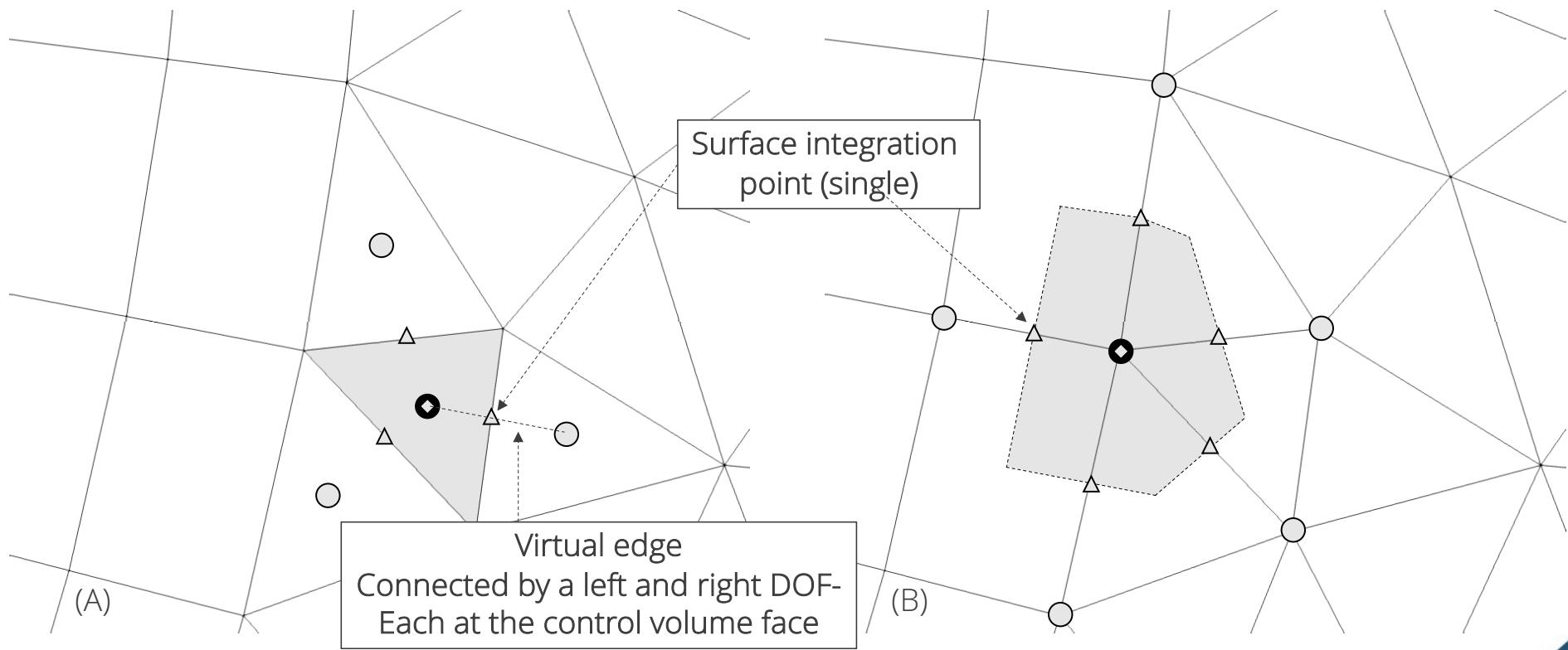
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Cell-Centered (CC) and Edge-Based Vertex-Centred (EBVC): Each are generally a two-state scheme, Left (L) and Right(R)

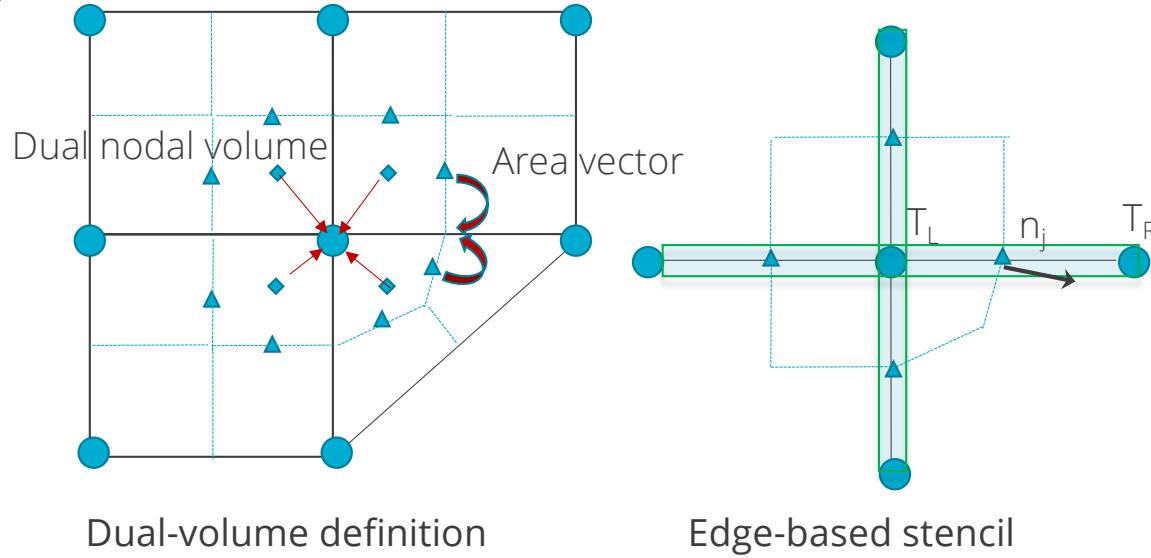
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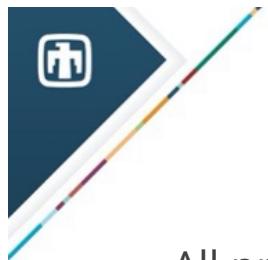




The Control Volume for EBVC is Defined by the **Dual-Volume**

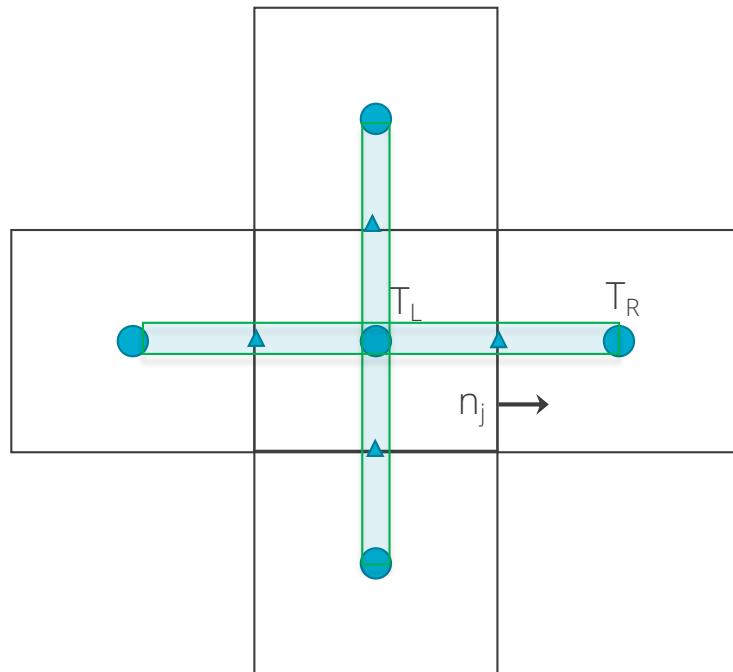
- All primitives are collocated at the vertices of the elements with equal-order interpolation
- A dual mesh is constructed to obtain flux and volume quadrature locations
- Classic two-state, “L” and “R” approach provides spatially second-order accuracy
- Iterate **Nodes** for volume-based contributions
- Iterate **Edges** for surface-based contributions





The Control Volume for CC is Defined by the ***Element Volume***

- All primitives are collocated at the cell-center of the element with equal-order interpolation
- Classic two-state, “L” and “R” approach provides spatially second-order accuracy
- Iterate ***Elements*** for volume-based contributions
- Iterate ***Virtual-Edges*** or ***Control Volume Faces*** for surface-based contributions





One-Dimensional Example of a Non-Uniform Mesh

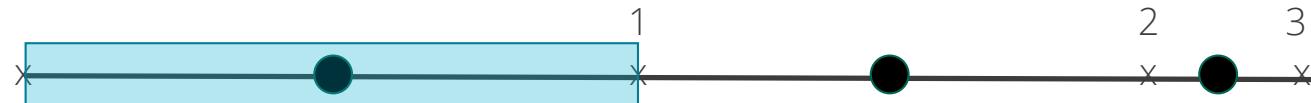
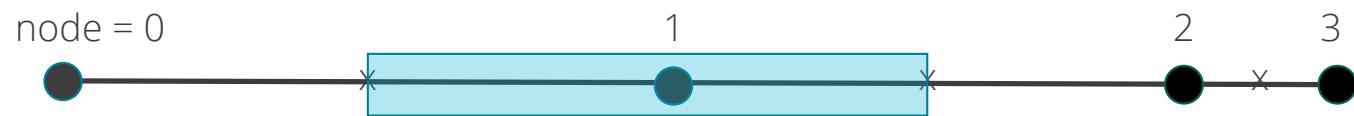
- The nodes of the mesh need-not be equally spaced





Control Volumes for CC and EBVC

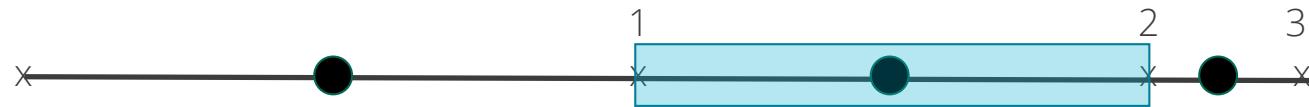
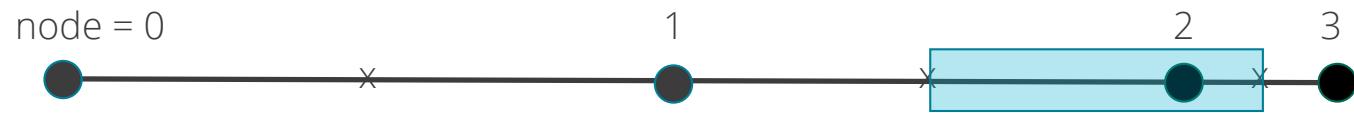
- Note: Switched depiction of node (or vertex) to the cell-centered location





Control Volumes for CC and EBVC

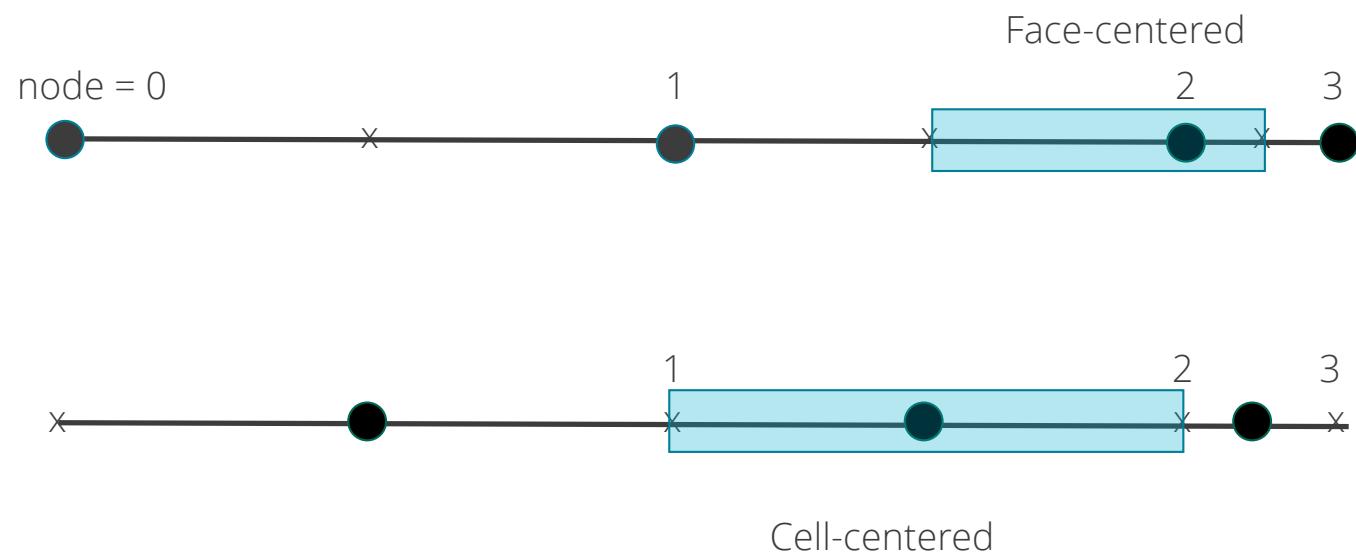
- Note: Switched depiction of node (or vertex) to the cell-centered location





Control Volumes for CC and EBVC

- Face-centered vs Cell-Centered





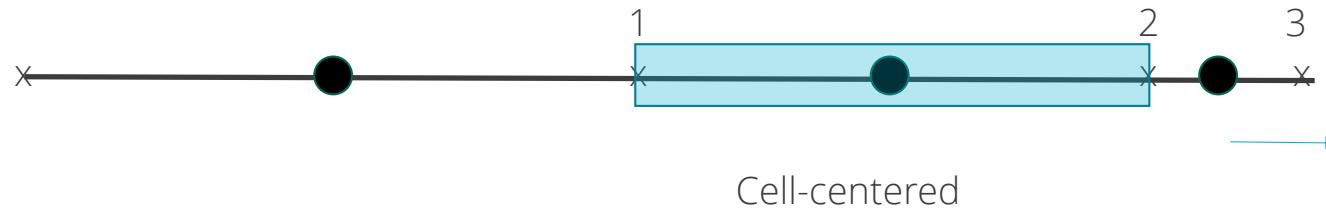
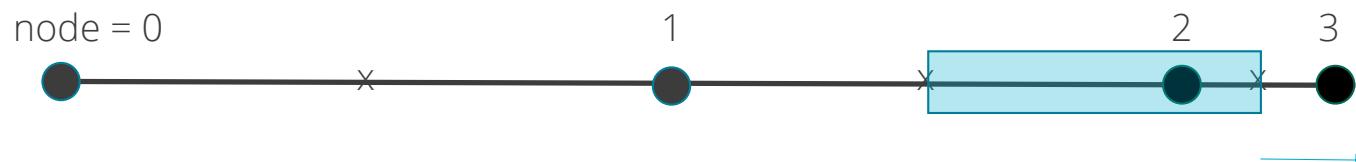
Basis Function Re-Visited

- Define an isoperimetric base element that varies from -1:+1, with integration point at the ξ location:

$$\phi_{ip} = \sum_n N_n^{ip} \phi_n$$

$$N_1 = \frac{(1 - \xi)}{2}$$

$$N_2 = \frac{(1 + \xi)}{2}$$



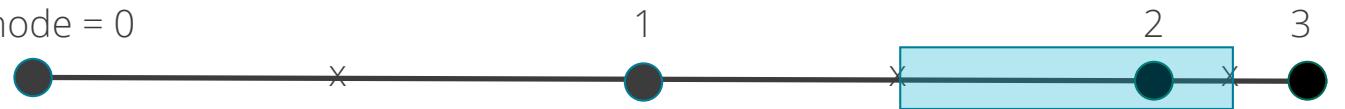


Basis Function Re-Visited

- Define an isoperimetric base element that varies from -1:+1, with integration point at the ξ location:

$$\phi_{ip} = \sum_n N_n^{ip} \phi_n$$

node = 0



Face-centered

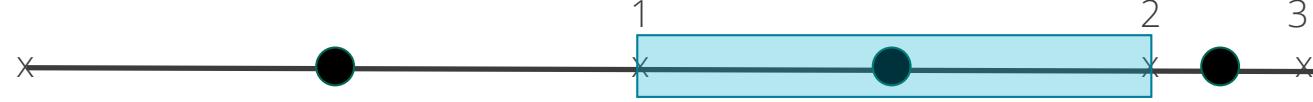
$$N_1 = \frac{(1 - \xi)}{2}$$

$$N_2 = \frac{(1 + \xi)}{2}$$

$2 \rightarrow 3$

$\xi = 0$

$$N_1 = N_2 = \frac{1}{2}$$



Cell-centered



Basis Function Re-Visited

- Define an isoperimetric base element that varies from -1:+1, with integration point at the ξ location:

$$\phi_{ip} = \sum_n N_n^{ip} \phi_n$$

$$N_1 = \frac{(1 - \xi)}{2}$$

$$N_2 = \frac{(1 + \xi)}{2}$$

node = 0



*

1

*

*

Face-centered

2

3

1

2

$2 \rightarrow 3$

$\xi = 0$

$$N_1 = N_2 = \frac{1}{2}$$

*

*

1

*

2

3

1

2

$1 \rightarrow 2$

$$N_1 = \frac{1}{4}; N_2 = \frac{3}{4} \quad \xi = 1/2$$

Cell-centered



Other Examples of a Basis (This will become important for the element-based schemes)

Linear (Quad4)

$$N_1 = \frac{1}{4}(1 - \xi)(1 - \eta)$$

$$N_2 = \frac{1}{4}(1 + \xi)(1 - \eta)$$

$$N_3 = \frac{1}{4}(1 + \xi)(1 + \eta)$$

$$N_4 = \frac{1}{4}(1 - \xi)(1 + \eta)$$

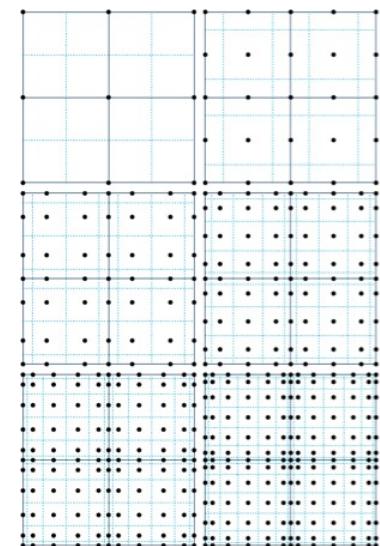
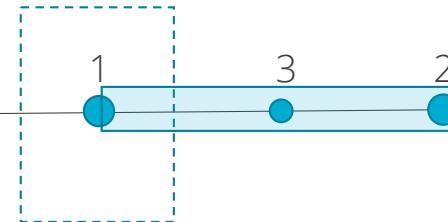
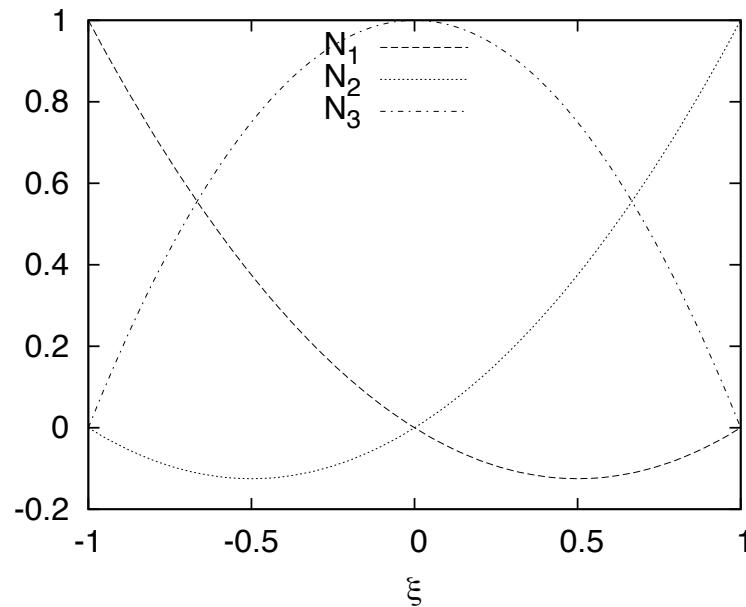
Quadratic (Bar3)

$$N_1 = \frac{-\xi(1 - \xi)}{2}$$

$$N_2 = \frac{\xi(1 + \xi)}{2}$$

$$N_3 = (1 - \xi)(1 + \xi)$$

$\widehat{\xi}$



Two-dimensional promotion



Simple One-D Diffusion Example

Let us introduce (briefly) the Method of Manufactured Solutions (MMS)

- Consider a simple diffusion equation:

$$\frac{d^2\phi}{dx^2} = 0$$

with a presumed, or manufactured solution:

$$\phi^{MMS}(x) = x^2$$

$$\frac{d^2\phi^{MMS}}{dx^2} = S^{MMS} = 2$$

Gauss-Divergence

$$\int \frac{d^2\phi^h}{dx^2} dV = \int S^{MMS} dV \quad \int \frac{d\phi^h}{dx} dS = \int S^{MMS} dV$$

Discrete flux-based form at the sub-control volume surface (scs) and sub-control volume IP:

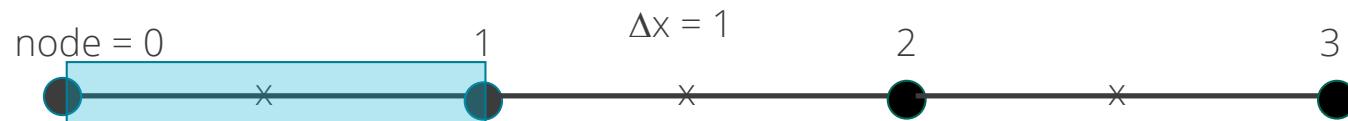
With error: $\epsilon = \phi^{MMS} - \phi^h$

$$\sum_{scsIP} \frac{d\phi^h}{dx} A_{scsIP} = \sum_{scvIP} S^{MMS} V_{scvIP}$$



Simple One-D MMS Example; Edge-based Assemble of Diffusion

We will use a linear basis and solve this system over a small patch of linear bar elements



Recall, simplified equation with RHS from source term already provided

$$\sum_{scsIP} \frac{d\phi^h}{dx}_{scsIP} = \sum_{scvIP} S^{MMS} \frac{\Delta x}{2}$$

Iterate elements with a simple left-hand side rule: $+= L$ and $-= R$
 (note implicit conservation statement)

$$\frac{d\phi^h}{dx}_{scsIP} = \frac{\phi_1^h - \phi_0^h}{\Delta x} + C_0(\Delta x) + \dots$$

$$LHS_0+ = \frac{\phi_1^h - \phi_0^h}{\Delta x}$$

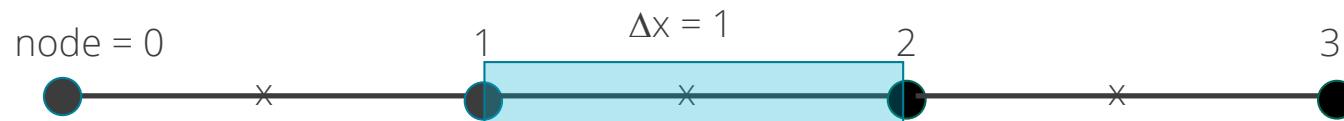
$$LHS_1- = \frac{\phi_1^h - \phi_0^h}{\Delta x}$$

Edge 1



Simple One-D MMS Example; Edge-based Assemble of Diffusion

We will use a linear basis and solve this system over a small patch of linear bar elements



Recall, simplified equation with RHS from source term already provided

$$\sum_{scsIP} \frac{d\phi^h}{dx}_{scsIP} = \sum_{scvIP} S^{MMS} \frac{\Delta x}{2}$$

Iterate elements with a simple left-hand side rule: $+= L$ and $-= R$
 (note implicit conservation statement)

$$\frac{d\phi^h}{dx}_{scsIP} = \frac{\phi_2^h - \phi_1^h}{\Delta x} + C_0(\Delta x) + \dots$$

$$LHS_1+ = \frac{\phi_2^h - \phi_1^h}{\Delta x}$$

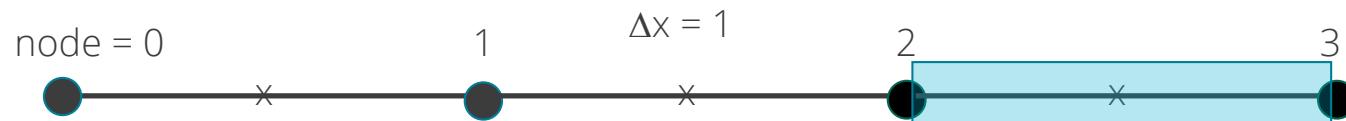
$$LHS_2- = \frac{\phi_2^h - \phi_1^h}{\Delta x}$$

Edge 2



Simple One-D MMS Example; Edge-based Assemble of Diffusion

We will use a linear basis and solve this system over a small patch of linear bar elements



Recall, simplified equation with RHS from source term already provided

$$\sum_{scsIP} \frac{d\phi^h}{dx}_{scsIP} = \sum_{scvIP} S^{MMS} \frac{\Delta x}{2}$$

Iterate elements with a simple left-hand side rule: += L and -=R

(note implicit conservation statement)

$$\frac{d\phi^h}{dx}_{scsIP} = \frac{\phi_3^h - \phi_2^h}{\Delta x} + C_0(\Delta x) + \dots$$

$$LHS_{2+} = \frac{\phi_3^h - \phi_2^h}{\Delta x}$$

$$LHS_{3-} = \frac{\phi_3^h - \phi_2^h}{\Delta x}$$

Edge 3



Simple One-D MMS Example; Collect all of the terms

$$LHS_0+ = \frac{\phi_1^h - \phi_0^h}{\Delta x}$$

$$LHS_1- = \frac{\phi_1^h - \phi_0^h}{\Delta x}$$

$$LHS_1+ = \frac{\phi_2^h - \phi_1^h}{\Delta x}$$

$$LHS_2- = \frac{\phi_2^h - \phi_1^h}{\Delta x}$$

$$LHS_2+ = \frac{\phi_3^h - \phi_2^h}{\Delta x}$$

$$LHS_3- = \frac{\phi_3^h - \phi_2^h}{\Delta x}$$

$$A = \frac{1}{\Delta x} \begin{bmatrix} -1 & +1 & 0 & 0 \\ +1 & -2 & +1 & 0 \\ 0 & +1 & -2 & 1 \\ 0 & 0 & +1 & -1 \end{bmatrix}$$

Fully assembled matrix

$$\frac{1}{\Delta x} \begin{bmatrix} -1 & +1 & 0 & 0 \\ +1 & -2 & +1 & 0 \\ 0 & +1 & -2 & 1 \\ 0 & 0 & +1 & -1 \end{bmatrix} \begin{bmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 2 \\ 2 \\ 2 \end{bmatrix}$$

Fully assembled system

$$\frac{1}{\Delta x} \begin{bmatrix} +1 & 0 & 0 & 0 \\ +1 & -2 & +1 & 0 \\ 0 & +1 & -2 & 1 \\ 0 & 0 & 0 & +1 \end{bmatrix} \begin{bmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 2 \\ 2 \\ 9 \end{bmatrix}$$

Correct for BCs

$$\phi^h = \begin{bmatrix} 0 \\ 1 \\ 4 \\ 9 \end{bmatrix}$$

Solution is exact.... Linear basis exactly captures a quadratic solution



Model Passive Scalar Transport: Introducing the Test Function, w

- Time/Src/Advection/Diffusion equation for scalar ϕ

$$\frac{\partial \rho\phi}{\partial t} + \frac{\partial \rho u_j \phi}{\partial x_j} - \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial \phi}{\partial x_j} \right) = S^\phi$$

Under the assumption, $\rho D = \frac{\mu}{Sc}$ yields: $\frac{\partial \rho\phi}{\partial t} + \frac{\partial \rho u_j \phi}{\partial x_j} - \frac{\partial}{\partial x_j} \left(\frac{\mu}{Sc} \frac{\partial \phi}{\partial x_j} \right) = S^\phi$

We can also integrate this PDE over the volume, while introducing a test function, w

$$\int w \left(\frac{\partial \rho\phi}{\partial t} + \frac{\partial}{\partial x_j} \left(\rho u_j \phi - \frac{\mu}{Sc} \frac{\partial \phi}{\partial x_j} \right) - S^\phi \right) dV = \int w R(\phi) dV$$

- The above is the so-called weak-form of the original (strong form) partial differential equation
- The elegant concept of a weighted residual statement is to seek a weak solution such that the residual is orthogonal to a selected space of weight functions



Model Passive Scalar Transport: Integration-by-Parts

- Recall, integration-by-parts, for example,

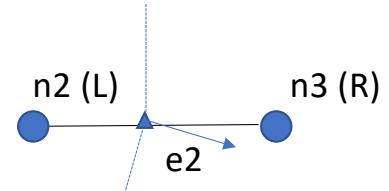
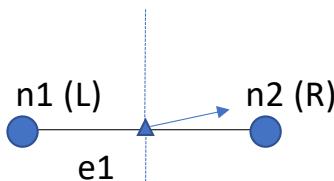
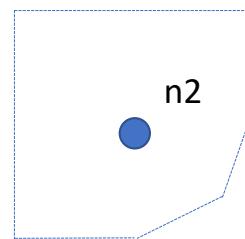
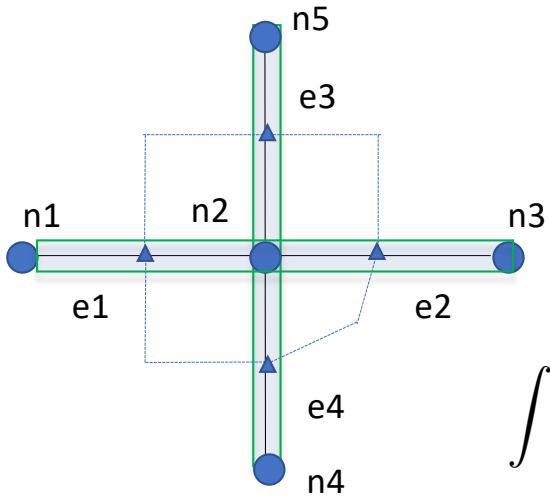
$$\int w \frac{\partial \rho u_j \phi}{\partial x_j} dV = - \int \rho u_j \phi \frac{\partial w}{\partial x_j} dV + \int w \rho u_j \phi n_j dS$$

- Note, that w must be differentiable at least once
- Under the special designation of w to be a piecewise constant, or Heaviside function, the gradient of this is a (negative) Diract-delta function
- A key property of this function is that the gradient of the piece-wise constant test function is a distribution of delta functions on the sub-control volume surface yielding,
$$\int \left(\frac{\partial \rho \phi}{\partial t} - S^\phi \right) dV + \int \left(\rho u_j \phi - \frac{\mu}{Sc} \frac{\partial \phi}{\partial x_j} \right) n_j dS = 0$$
- Recall, we could have arrived at this form by simply usage of Gauss-Divergence, however, this formality allows us to view a finite volume scheme as a Petrov-Galerkin scheme, i.e., the underlying basis differs from the test function

Deep Dive on EBVC: Node and Edge-loops

EBVC is a discretization scheme that:

- Uses a piecewise-constant test function
- Is a two-state flux approach, with a face-centered arrangement
- Iterates over locally-owned nodes for Time/Source/etc. (volumetric-based terms)
- Iterates over locally-owned edges for Advection/Diffusion terms (surface-based terms)



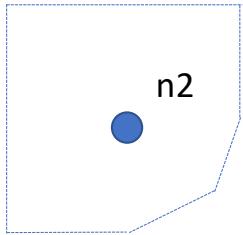
$$\int w S^\phi dV \approx \sum_{nd} S_{nd}^\phi V_{nd}$$

$$\int w \frac{\partial \rho u_j \phi}{\partial x_j} dV \approx \sum_{ip} (\rho u_j)_{ip} \phi_{ip} n_j dS \approx \sum_{ip} \dot{m}_{ip} \phi_{ip}$$

EBVC: Implicit Time Discretization

- Let us define a general implicit time integrator that is A-stable
 - For $y' = k y$; $y(0) = 1$; $y(t) = e^{kt}$ solution approaches zero as time increases for $k < 0$
- Backward Euler (two state) and is first-order accurate (A-stable)
- BDF2 (three state) is second-order accurate (A-stable)

This term is assembled over a nodal iteration and uses a single integration point (known as mass-lumping)


$$\int w \frac{\partial \rho \phi}{\partial t} dV \approx \sum_{nd} \frac{(\gamma_1 \rho_{nd}^{n+1} + \gamma_1 \rho_{nd}^n + \gamma_1 \rho_{nd}^{n-1})}{\Delta t} V_{nd}$$

For uniform time stepping, the coefficients are given by, $\gamma_1 = 3/2$ $\gamma_2 = -2$ $\gamma_3 = 1/2$



EBVC: Implicit Time Discretization; Code

- <https://github.com/NaluCFD/Nalu/blob/master/src/ScalarMassBDF2NodeSuppAlg.C>

```
//-----
//----- node_execute -----
//-----
void
ScalarMassBDF2NodeSuppAlg::node_execute(
    double *lhs,
    double *rhs,
    stk::mesh::Entity node)
{
    // deal with lumped mass matrix
    const double qNm1      = *stk::mesh::field_data(*scalarQNm1_, node);
    const double qN          = *stk::mesh::field_data(*scalarQN_, node);
    const double qNp1        = *stk::mesh::field_data(*scalarQNp1_, node);
    const double rhoNm1     = *stk::mesh::field_data(*densityNm1_, node);
    const double rhoN        = *stk::mesh::field_data(*densityN_, node);
    const double rhoNp1      = *stk::mesh::field_data(*densityNp1_, node);
    const double dualVolume = *stk::mesh::field_data(*dualNodalVolume_, node);
    const double lhsTime     = gamma1_*rhoNp1*dualVolume/dt_;
    rhs[0] -= (gamma1_*rhoNp1*qNp1 + gamma2_*qN*rhoN + gamma3_*qNm1*rhoNm1)*dualVolume/dt_;
    lhs[0] += lhsTime;
}
```

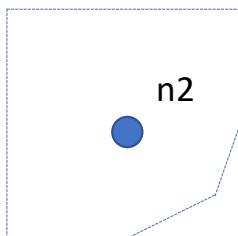


EBVC: Source Term Discretization

- Source terms for the edge-based scheme are also assembled over a nodal loop
- Note that in this scheme, we are using single point quadrature, i.e., the function is evaluated at a single point

The single point integration point leverages the fact that: $p = 2N - 1$

- Where N is the number of integration points and p is the polynomial order
- For a linear basis, using one-point quadrature is design-order, or second-order in space



$$\int w S^\phi dV \approx \sum_{nd} S_{nd}^\phi V_{nd}$$



EBVC: Source Term Discretization; Code

- https://github.com/NaluCFD/Nalu/blob/master/src/user_functions/VariableDensityMixFracSrcNodeSuppAlg.C

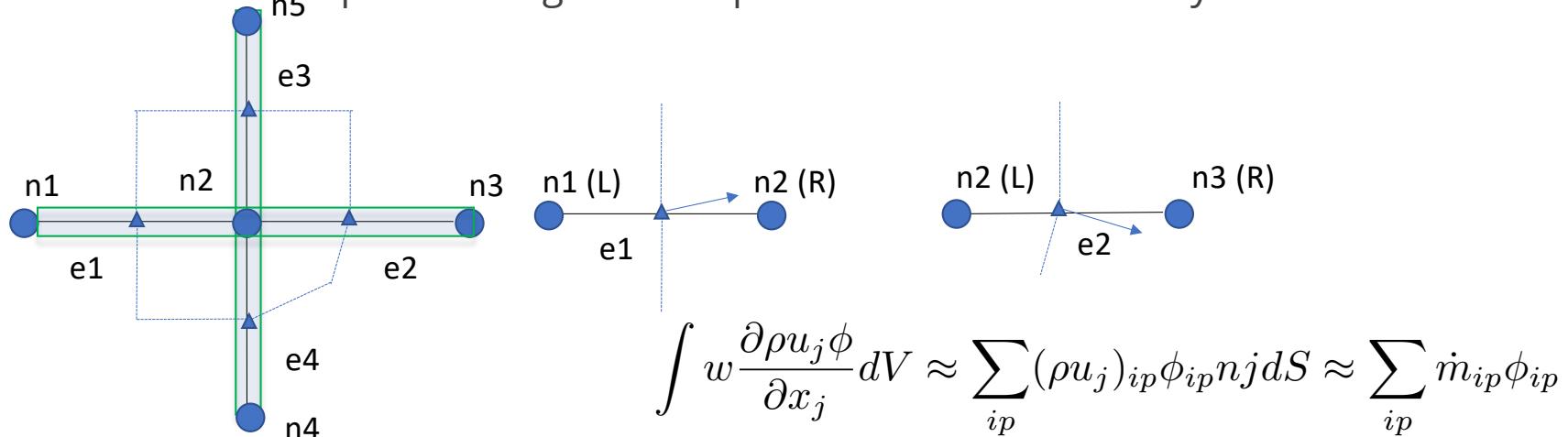
```
//-----
//----- node_execute -----
//-----
void
VariableDensityMixFracSrcNodeSuppAlg::node_execute(
    double /*lhs*/,
    double *rhs,
    stk::mesh::Entity node)
{
    // deal with lumped mass matrix
    const double *coords = stk::mesh::field_data(*coordinates_, node);
    const double dualVolume = *stk::mesh::field_data(*dualNodalVolume_, node );
    const double x = coords[0];
    const double y = coords[1];
    const double z = coords[2];

    const double src = 0.10e1 * pow(znot_ * cos(amf_ * pi_ * x) * cos(amf_ * pi_ * y) * cos(amf_
        rhs[0] += src*dualVolume;
}
```



EBVC: Advection Term Discretization

- For advection, we have transformed the volume integral to a surface integration
- Therefore, a patch of edges are required for the full assembly at node 2



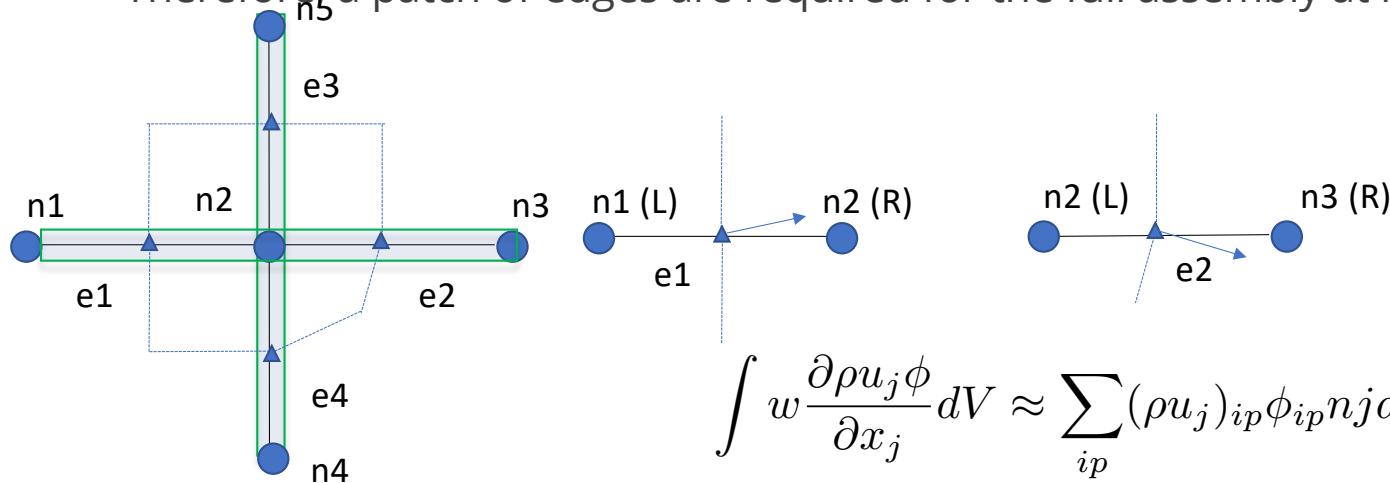
- Recall, that the mass flow rate at an integration point is prescribed
- Moreover, since the integration point is at the edge mid-point, $\phi_{ip} = (\phi^R + \phi^L)/2$

This is a *central-* or *Galerkin-based* advection operator; shown in conservative form, i.e, is in divergence form and has been integrated-by-parts



EBVC: Advection Term Discretization

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$$\int w \frac{\partial \rho u_j \phi}{\partial x_j} dV \approx \sum_{ip} (\rho u_j)_{ip} \phi_{ip} n_j dS \approx \sum_{ip} \dot{m}_{ip} \phi_{ip}$$

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This is a *central-* or *Galerkin-based* advection operator; shown in conservative form, i.e, is in divergence form and has been integrated-by-parts

Mahesh et al., JCP (2004)

For kinetic energy conservation, a CC scheme also uses $\frac{1}{2}$ weights!



EBVC: Advection Term Discretization; Code

- <https://github.com/NaluCFD/Nalu/blob/master/src/AssembleScalarEdgeSolverAlgorithm.C>



Upwind Advection Operators

- Recall from our finite difference class that in absence of a stabilizing diffusion term, or when the velocity is very high, i.e., the Peclet number > 2, non-physical oscillations can be noted
- An upwind approach was devised to mitigate this at the expense of numerical accuracy
- For a finite volume approach, upwinding is very easy to construct



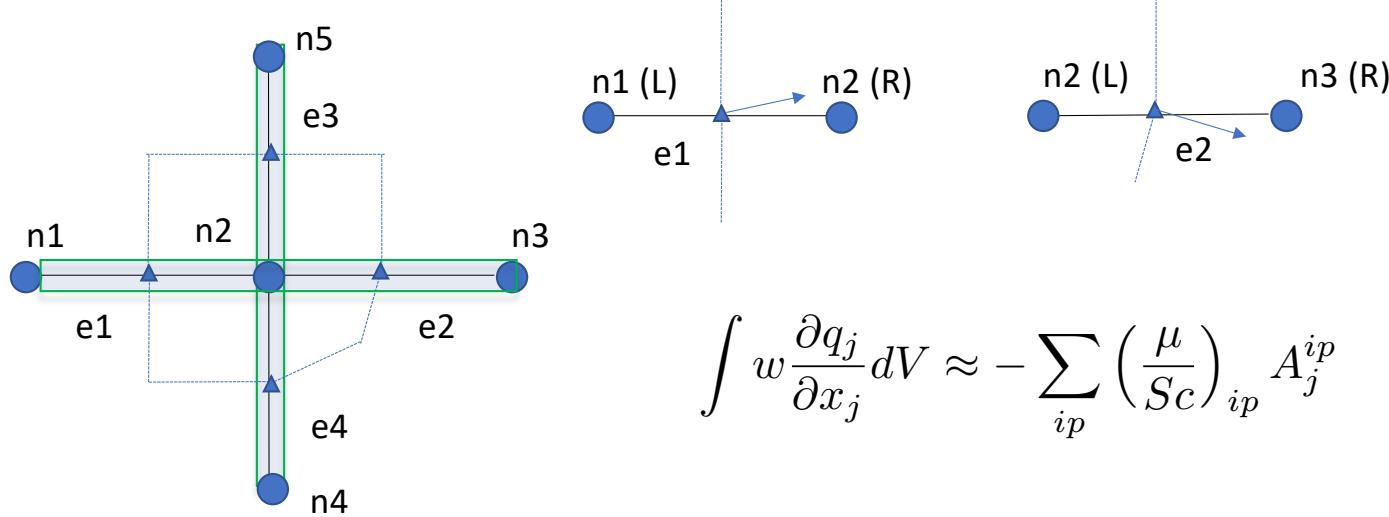
$$\phi_{j+1/2} = \begin{cases} \phi_j, & \text{if } u_l n_l > 0. \\ \phi_{j+1}, & \text{otherwise.} \end{cases} \quad \text{"as the wind blows"}$$

- However, upwind operators, even if higher-order, are numerically dissipative due to loss of symmetry of the operator
- Higher-order upwind (second-order in space) can be obtained on an unstructured mesh by use of projected nodal gradients and extrapolation (will cover this in the advection operator section)



EBVC: Diffusion

- For diffusion, we have transformed the volume integral to a surface integration
- Therefore, a patch of edges are required for the full assembly at node 2

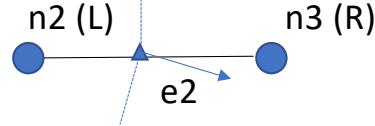




EBVC: Diffusion, Non-Orthogonality

- The edge-based diffusion operator is a bit more complex in that we are computing a gradient at the integration point while using two nodes, the left and right
- In many practical meshes, the distance vector between the edges (\mathbf{dx}_j) and the edge area vector will not be perfectly orthogonal
- This non-orthogonality causes inaccuracy when using a simplified approach

$$\frac{\partial \phi}{\partial x_j} = \frac{(\phi_R - \phi_L)}{|\Delta x_l|} n_j$$



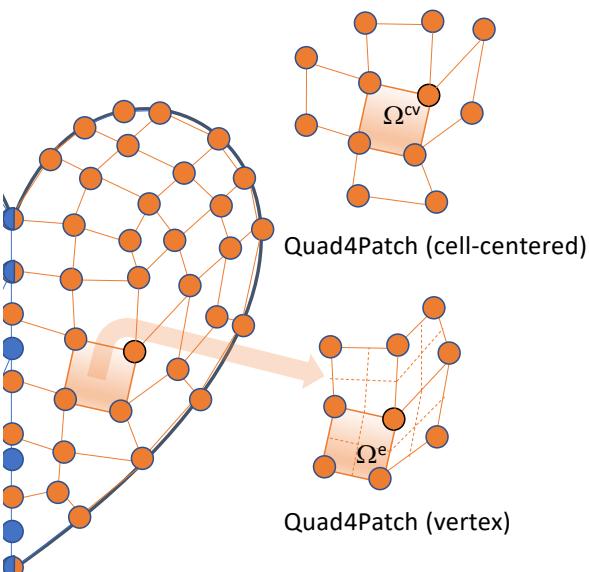
- The non-orthogonality approach of Jasek (Ph.D. Imperial College) is a standard cell-centered approach that has been adopted for edge-based schemes
- CC and EBVC are each two-state schemes and share non-orthogonality issues

$$\left. \frac{\partial \phi}{\partial x_j} \right|_{ip} = \overline{G_j \phi} + [(\phi_R - \phi_L) - \overline{G_l \phi} \Delta x_l] \frac{A_j}{A_k \Delta x_k}$$

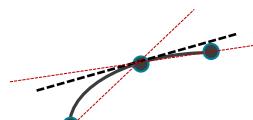
Where $G_j \phi$ is a “projected nodal gradient”

(Projected) Nodal Gradient Operator

- Recall, that the edge-based diffusion operator, and as we will see in future lectures for some choices for the advection operator, a nodal gradient is required



- First, the gradient of a function (other than linear) is discontinuous, i.e., the value at a shared element face depends on which element is used to compute the gradient
- Therefore, we can view the nodal gradient a continuous at the nodes and discontinuous within the elements



Let's minimize this difference: $\frac{1}{2} \left(\frac{\partial \phi}{\partial x_j} - G_j \phi \right)^2$
by solving:

$$\int w G_j \phi dV = \int w \frac{\partial \phi}{\partial x_j} dV \longrightarrow G_j \phi = \frac{\sum_{ip} \phi_{ip} n_j dS}{V}$$



EBVC: Diffusion, Non-Orthogonality; Code

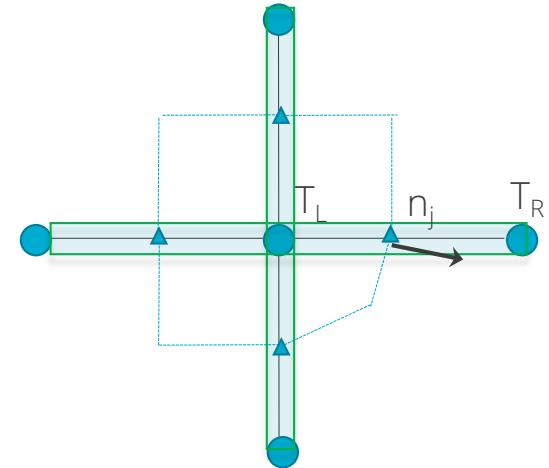
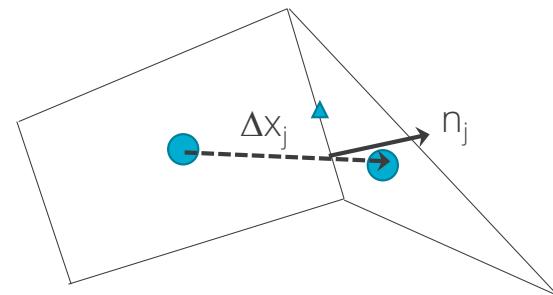
- <https://github.com/NaluCFD/Nalu/blob/master/src/AssembleScalarEdgeDiffSolverAlgorithm.C>

$$-\int w \frac{\mu}{Sc} \frac{\partial \phi}{\partial x_j} dV \approx - \left. \frac{\mu}{Sc} \right|_{ip} \left[(\overline{G_x \phi} A_x + \overline{G_y \phi} A_y) + (\phi_R - \phi_L) \frac{A_x A_x + A_y A_y}{A_x \Delta x_x + A_y \Delta x_y} - (\overline{G_x \phi} dx + \overline{G_y \phi} dy) \frac{A_x A_x + A_y A_y}{A_x dx + A_y dy} \right]$$



Typical Difficulties for a Two-State Scheme

- With two points, only a linear basis can be used, therefore, unstructured CC and EBVC are limited to second-order spatial accuracy
- Non-orthogonality, or the mis-alignment of the distance vector between the two "L" and "R" states and the surface normal, is present
- Integration point
- Both edge- and cell centered-based schemes show degraded accuracy on typical production meshes
- Several non-orthogonality approaches are available, for the best source, see Jasak
 - Jasak, "Error analysis and error estimation for the finite volume method with applications to fluid flow", Imperial College Dissertation, 1996





For Instance, Verification of The Diffusion Operator

